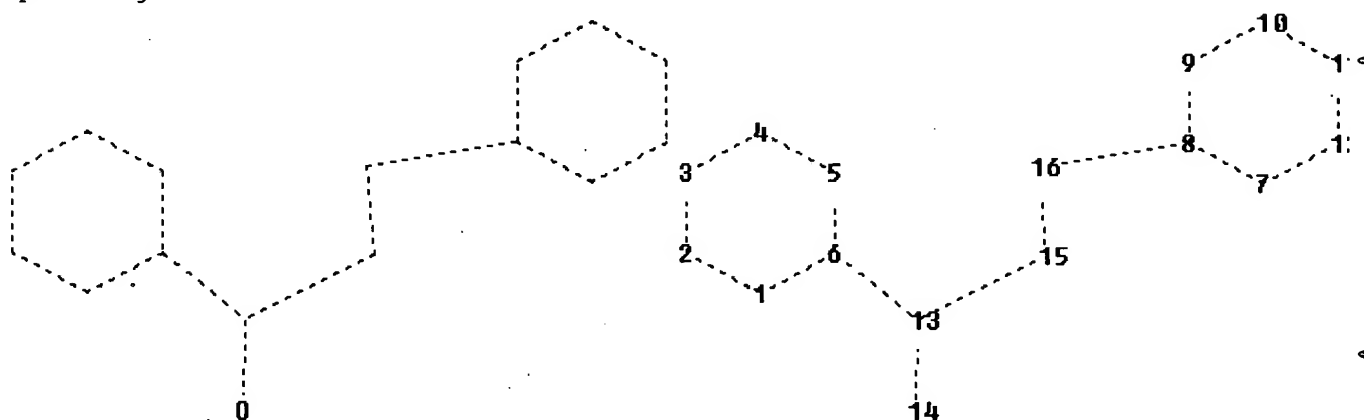


Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str



chain nodes :

13 14 15 16

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

6-13 8-16 13-14 13-15 15-16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 6-13 7-8 7-12 8-9 8-16 9-10 10-11 11-12 13-14
13-15 15-16

Connectivity :

1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC
ring/chain

4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
7:3 X maximum

RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X
maximum RC ring/chain

11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC
ring/chain 14:1

E exact RC ring/chain 15:3 X maximum RC ring/chain 16:3 X maximum RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS

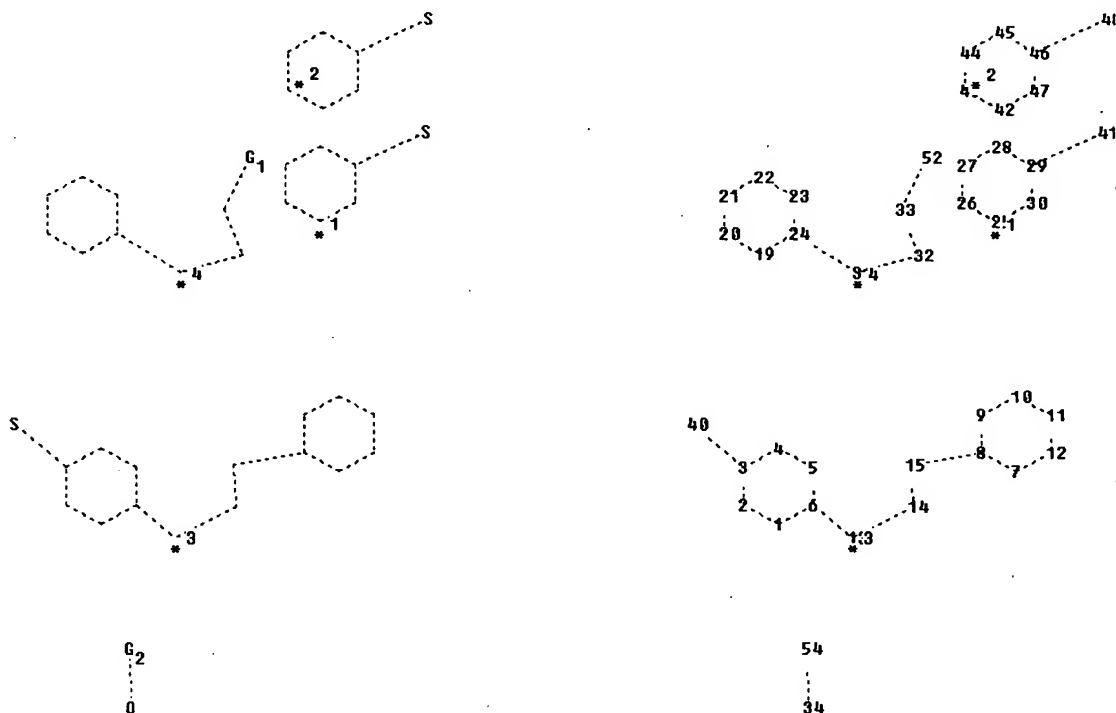
L3

STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:

Uploading L3.str



chain nodes :

13 14 15 31 32 33 34 40 41 48 52 54

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 19 20 21 22 23 24 25 26 27 28 29
30 42 43 44 45 46 47

chain bonds :

3-40 6-13 8-15 13-14 14-15 24-31 29-41 31-32 32-33 33-52 34-54 46-48

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24 20-21
21-22 22-23 23-24 25-26 25-30 26-27 27-28 28-29 29-30 42-43 42-47 43-44
44-45 45-46
46-47

exact/norm bonds :

1-2 1-6 2-3 3-4 3-40 4-5 5-6 6-13 7-8 7-12 8-9 8-15 9-10 10-11 11-12
13-14 14-15 19-20 19-24 20-21 21-22 22-23 23-24 24-31 25-26 25-30 26-27
27-28 28-29

10/520079

29-30 29-41 31-32 32-33 33-52 34-54 42-43 42-47 43-44 44-45 45-46 46-47
46-48

G1:[*1],[*2]

G2:[*3],[*4]

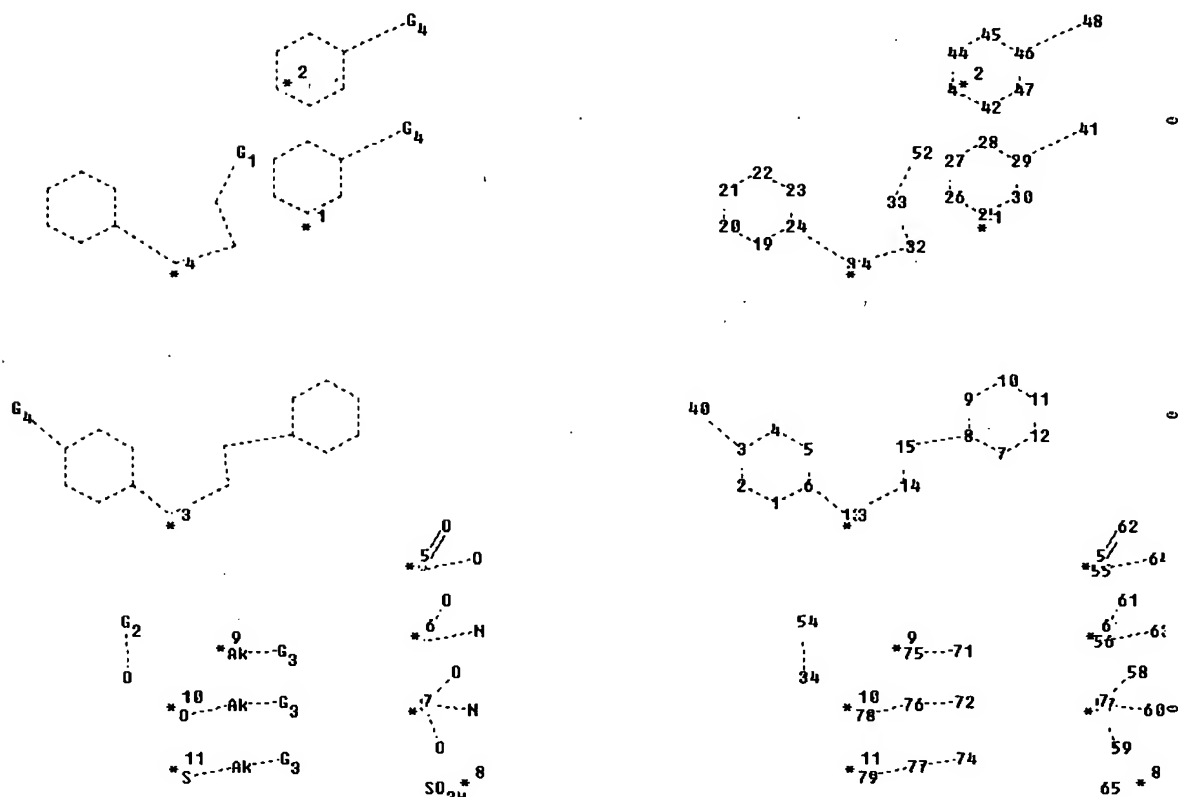
Connectivity :

1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC
ring/chain
4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
7:3 X maximum
RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X
maximum RC ring/chain
11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC
ring/chain 14:3
X maximum RC ring/chain 15:3 X maximum RC ring/chain 19:3 X maximum RC ring/chain
20:3 X maximum
RC ring/chain 21:3 X maximum RC ring/chain 22:3 X maximum RC ring/chain 23:3 X
maximum RC ring/chain
24:3 E exact RC ring/chain 25:3 X maximum RC ring/chain 26:3 X maximum RC
ring/chain 27:3
X maximum RC ring/chain 28:3 X maximum RC ring/chain 29:3 X maximum RC ring/chain
30:3 X maximum
RC ring/chain 31:3 E exact RC ring/chain 32:3 X maximum RC ring/chain 33:3 X
maximum RC ring/chain
34:1 E exact RC ring/chain 42:3 X maximum RC ring/chain 43:3 X maximum RC
ring/chain 44:3
X maximum RC ring/chain 45:3 X maximum RC ring/chain 47:3 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS
34:CLASS 40:CLASS
41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 52:CLASS
54:CLASS

L5 2322 SEA FILE=REGISTRY SSS FUL L3 AND L1
L6 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation:
Uploading L6.str



chain nodes :

13 14 15 31 32 33 34 40 41 48 52 54 55 56 57 58 59 61 62 64 65
71 72 74 75 76 77 78 79

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 19 20 21 22 23 24 25 26 27 28 29
30 42 43 44 45 46 47

ring/chain nodes :

60 63

chain bonds :

3-40 6-13 8-15 13-14 14-15 24-31 29-41 31-32 32-33 33-52 34-54 46-48
55-62 55-64 56-61 56-63 57-58 57-59 57-60 71-75 72-76 74-77 76-78 77-79

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24 20-21

21-22 22-23 23-24 25-26 25-30 26-27 27-28 28-29 29-30 42-43 42-47 43-44
44-45 45-46

46-47

exact/norm bonds :

1-2 1-6 2-3 3-4 3-40 4-5 5-6 6-13 7-8 7-12 8-9 8-15 9-10 10-11 11-12
13-14 14-15 19-20 19-24 20-21 21-22 22-23 23-24 24-31 25-26 25-30 26-27

27-28 28-29

29-30 29-41 31-32 32-33 33-52 34-54 42-43 42-47 43-44 44-45 45-46 46-47

46-48 55-62

55-64 56-61 56-63 57-58 57-59 57-60 71-75 72-76 74-77 76-78 77-79

G1:[*1],[*2]

G2:[*3],[*4]

G3:[*5],[*6],[*7],[*8]

G4:[*9],[*10],[*11]

Connectivity :

1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC ring/chain
 4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
 7:3 X maximum RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X maximum RC ring/chain
 11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC ring/chain 14:3 X maximum RC ring/chain
 15:3 X maximum RC ring/chain 19:3 X maximum RC ring/chain 20:3 X maximum RC ring/chain
 21:3 X maximum RC ring/chain 22:3 X maximum RC ring/chain 23:3 X maximum RC ring/chain
 24:3 E exact RC ring/chain 25:3 X maximum RC ring/chain 26:3 X maximum RC ring/chain 27:3 X maximum RC ring/chain
 28:3 X maximum RC ring/chain 29:3 X maximum RC ring/chain 30:3 X maximum RC ring/chain
 31:3 E exact RC ring/chain 32:3 X maximum RC ring/chain 33:3 X maximum RC ring/chain
 34:1 E exact RC ring/chain 42:3 X maximum RC ring/chain 43:3 X maximum RC ring/chain 44:3 X maximum RC ring/chain
 45:3 X maximum RC ring/chain 47:3 X maximum RC ring/chain

Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom
 23:Atom 24:Atom
 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS
 34:CLASS 40:CLASS
 41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 52:CLASS
 54:CLASS
 55:CLASS 56:CLASS 57:CLASS 58:CLASS 59:CLASS 60:CLASS 61:CLASS 62:CLASS
 63:CLASS 64:CLASS
 65:CLASS 71:CLASS 72:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS 78:CLASS
 79:CLASS

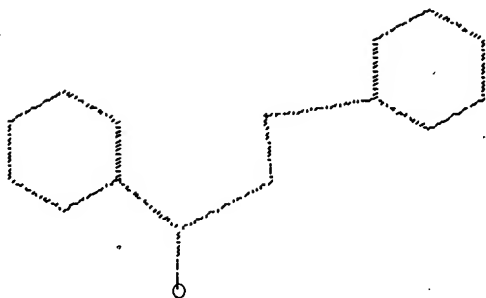
L8 68 SEA FILE=REGISTRY SUB=L5 SSS FUL L6
 L9 12 SEA FILE=ZCAPLUS ABB=ON PLU=ON L8
 L18 2 SEA FILE=ZCAPLUS ABB=ON PLU=ON US2005-520079 /APPS
 L19 2 SEA FILE=ZCAPLUS ABB=ON PLU=ON L18 AND L9

=> d stat que L23

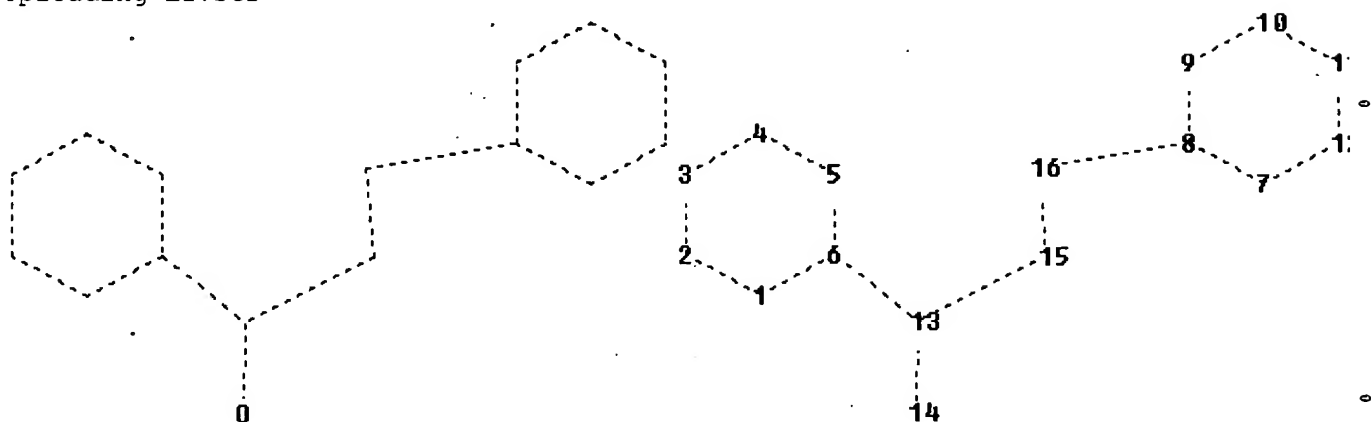
L20 38 SEA FILE=ZCAPLUS ABB=ON PLU=ON NAJIB J?/AU
 L21 70 SEA FILE=ZCAPLUS ABB=ON PLU=ON CAUMONT K?/AU OR BERTRAND
 K?/AU
 L22 11 SEA FILE=ZCAPLUS ABB=ON PLU=ON CAUMONT B?/AU
 L23 5 SEA FILE=ZCAPLUS ABB=ON PLU=ON L20 AND (L21 OR L22)

=> d stat que L24

L1 STR



Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str



chain nodes :

13 14 15 16

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

6-13 8-16 13-14 13-15 15-16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 6-13 7-8 7-12 8-9 8-16 9-10 10-11 11-12 13-14
13-15 15-16

Connectivity :

1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC ring/chain

4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain 7:3 X maximum

RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X maximum RC ring/chain

11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC ring/chain 14:1

E exact RC ring/chain 15:3 X maximum RC ring/chain 16:3 X maximum RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

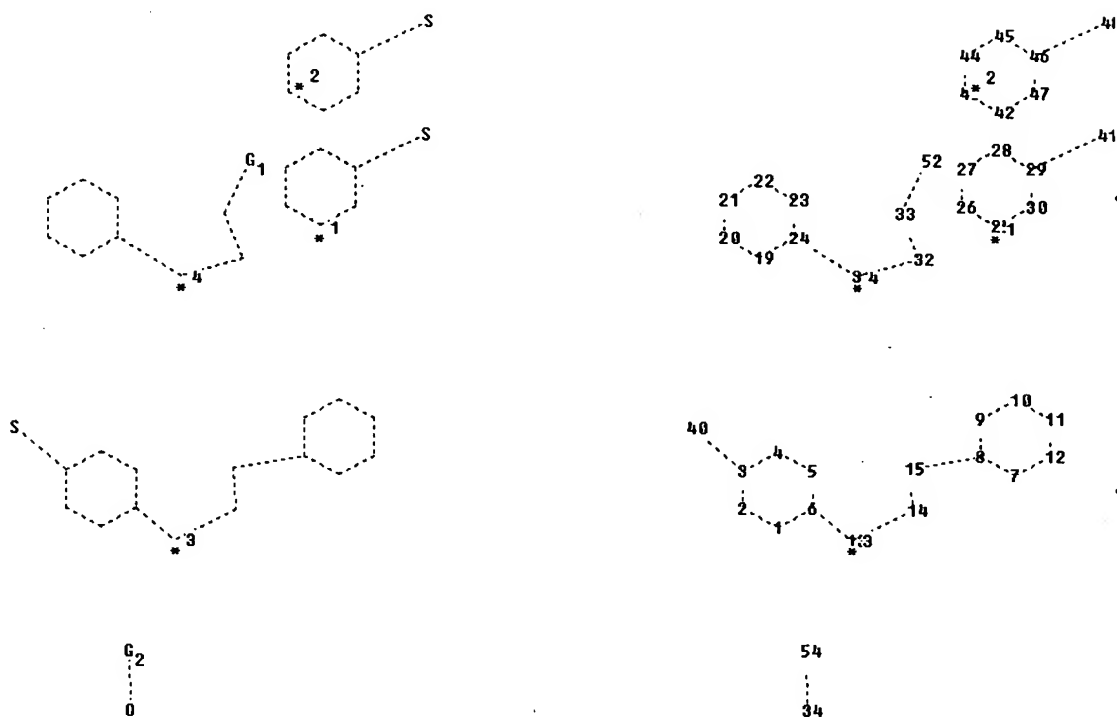
10/520079

11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS

L3 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L3.str



chain nodes :

13 14 15 31 32 33 34 40 41 48 52 54

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 19 20 21 22 23 24 25 26 27 28 29
30 42 43 44 45 46 47

chain bonds :

3-40 6-13 8-15 13-14 14-15 24-31 29-41 31-32 32-33 33-52 34-54 46-48

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24 20-21
21-22 22-23 23-24 25-26 25-30 26-27 27-28 28-29 29-30 42-43 42-47 43-44
44-45 45-46
46-47

exact/norm bonds :

1-2 1-6 2-3 3-4 3-40 4-5 5-6 6-13 7-8 7-12 8-9 8-15 9-10 10-11 11-12
13-14 14-15 19-20 19-24 20-21 21-22 22-23 23-24 24-31 25-26 25-30 26-27

10/520079

27-28 28-29
29-30 29-41 31-32 32-33 33-52 34-54 42-43 42-47 43-44 44-45 45-46 46-47
46-48

G1:[*1],[*2]

G2:[*3],[*4]

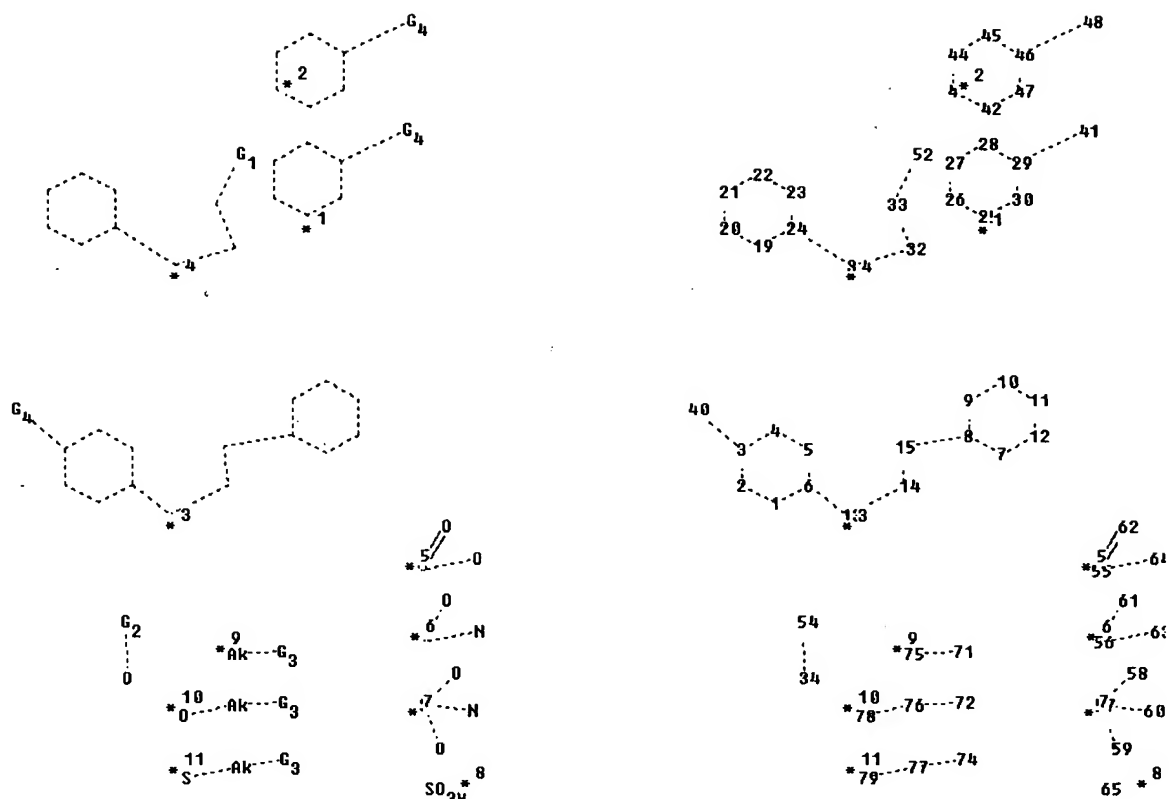
Connectivity :

1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC ring/chain
4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
7:3 X maximum RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X maximum RC ring/chain
11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC ring/chain 14:3 X maximum RC ring/chain
15:3 X maximum RC ring/chain 19:3 X maximum RC ring/chain 20:3 X maximum RC ring/chain
21:3 X maximum RC ring/chain 22:3 X maximum RC ring/chain 23:3 X maximum RC ring/chain
24:3 E exact RC ring/chain 25:3 X maximum RC ring/chain 26:3 X maximum RC ring/chain 27:3 X maximum RC ring/chain
28:3 X maximum RC ring/chain 29:3 X maximum RC ring/chain 30:3 X maximum RC ring/chain
31:3 E exact RC ring/chain 32:3 X maximum RC ring/chain 33:3 X maximum RC ring/chain
34:1 E exact RC ring/chain 42:3 X maximum RC ring/chain 43:3 X maximum RC ring/chain 44:3 X maximum RC ring/chain
45:3 X maximum RC ring/chain 47:3 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS
34:CLASS 40:CLASS
41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 52:CLASS
54:CLASS

L5 2322 SEA FILE=REGISTRY SSS FUL L3 AND L1
L6 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation:
Uploading L6.str



chain nodes :

13 14 15 31 32 33 34 40 41 48 52 54 55 56 57 58 59 61 62 64 65
71 72 74 75 76 77 78 79

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 19 20 21 22 23 24 25 26 27 28 29
30 42 43 44 45 46 47

ring/chain nodes :

60 63

chain bonds :

3-40 6-13 8-15 13-14 14-15 24-31 29-41 31-32 32-33 33-52 34-54 46-48
55-62 55-64 56-61 56-63 57-58 57-59 57-60 71-75 72-76 74-77 76-78 77-79

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24 20-21

21-22 22-23 23-24 25-26 25-30 26-27 27-28 28-29 29-30 42-43 42-47 43-44
44-45 45-46

46-47

exact/norm bonds :

1-2 1-6 2-3 3-4 3-40 4-5 5-6 6-13 7-8 7-12 8-9 8-15 9-10 10-11 11-12
13-14 14-15 19-20 19-24 20-21 21-22 22-23 23-24 24-31 25-26 25-30 26-27

27-28 28-29

29-30 29-41 31-32 32-33 33-52 34-54 42-43 42-47 43-44 44-45 45-46 46-47

46-48 55-62

55-64 56-61 56-63 57-58 57-59 57-60 71-75 72-76 74-77 76-78 77-79

G1:[*1],[*2]

=> file registry

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STRUCTURE FILE UPDATES: 30 SEP 2007 HIGHEST RN 948879-65-0
DICTIONARY FILE UPDATES: 30 SEP 2007 HIGHEST RN 948879-65-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> file zcaplus

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FILE COVERS 1907 - 1 Oct 2007 VOL 147 ISS 15
FILE LAST UPDATED: 30 Sep 2007 (20070930/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

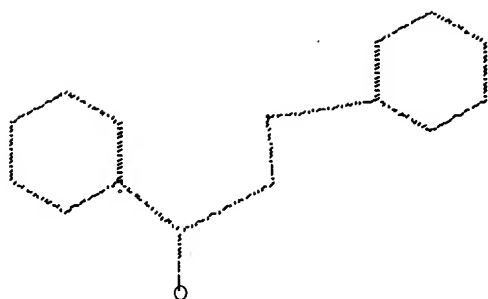
This file contains CAS Registry Numbers for easy and accurate
substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

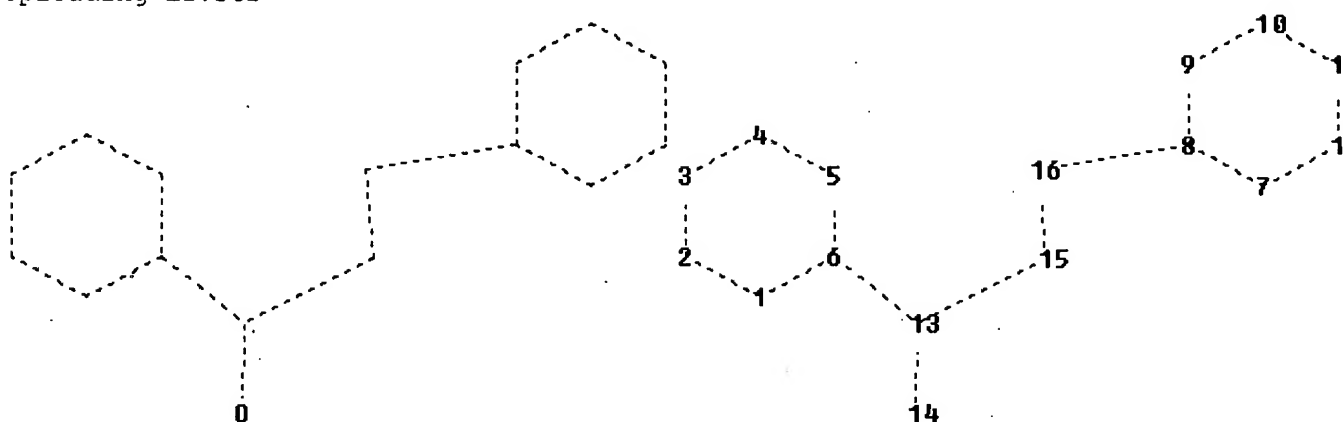
=> d stat que L19

L1 STR

10/520079



Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str



chain nodes :

13 14 15 16

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

6-13 8-16 13-14 13-15 15-16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 6-13 7-8 7-12 8-9 8-16 9-10 10-11 11-12 13-14
13-15 15-16

Connectivity :

1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC
ring/chain

4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
7:3 X maximum

RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X
maximum RC ring/chain

11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC
ring/chain 14:1

E exact RC ring/chain 15:3 X maximum RC ring/chain 16:3 X maximum RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS

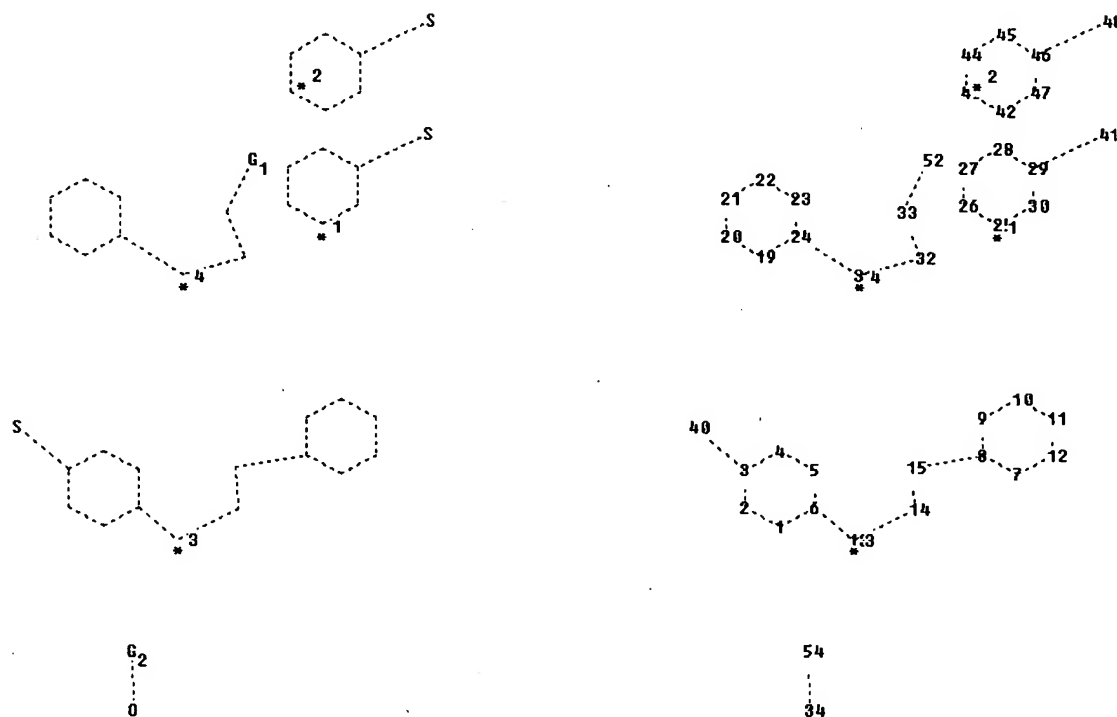
L3

STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:

Uploading L3.str



chain nodes :

13 14 15 31 32 33 34 40 41 48 52 54

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 19 20 21 22 23 24 25 26 27 28 29
30 42 43 44 45 46 47

chain bonds :

3-40 6-13 8-15 13-14 14-15 24-31 29-41 31-32 32-33 33-52 34-54 46-48

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24 20-21
21-22 22-23 23-24 25-26 25-30 26-27 27-28 28-29 29-30 42-43 42-47 43-44
44-45 45-46
46-47

exact/norm bonds :

1-2 1-6 2-3 3-4 3-40 4-5 5-6 6-13 7-8 7-12 8-9 8-15 9-10 10-11 11-12
13-14 14-15 19-20 19-24 20-21 21-22 22-23 23-24 24-31 25-26 25-30 26-27
27-28 28-29

10/520079

29-30 29-41 31-32 32-33 33-52 34-54 42-43 42-47 43-44 44-45 45-46 46-47
46-48

G1:[*1],[*2]

G2:[*3],[*4]

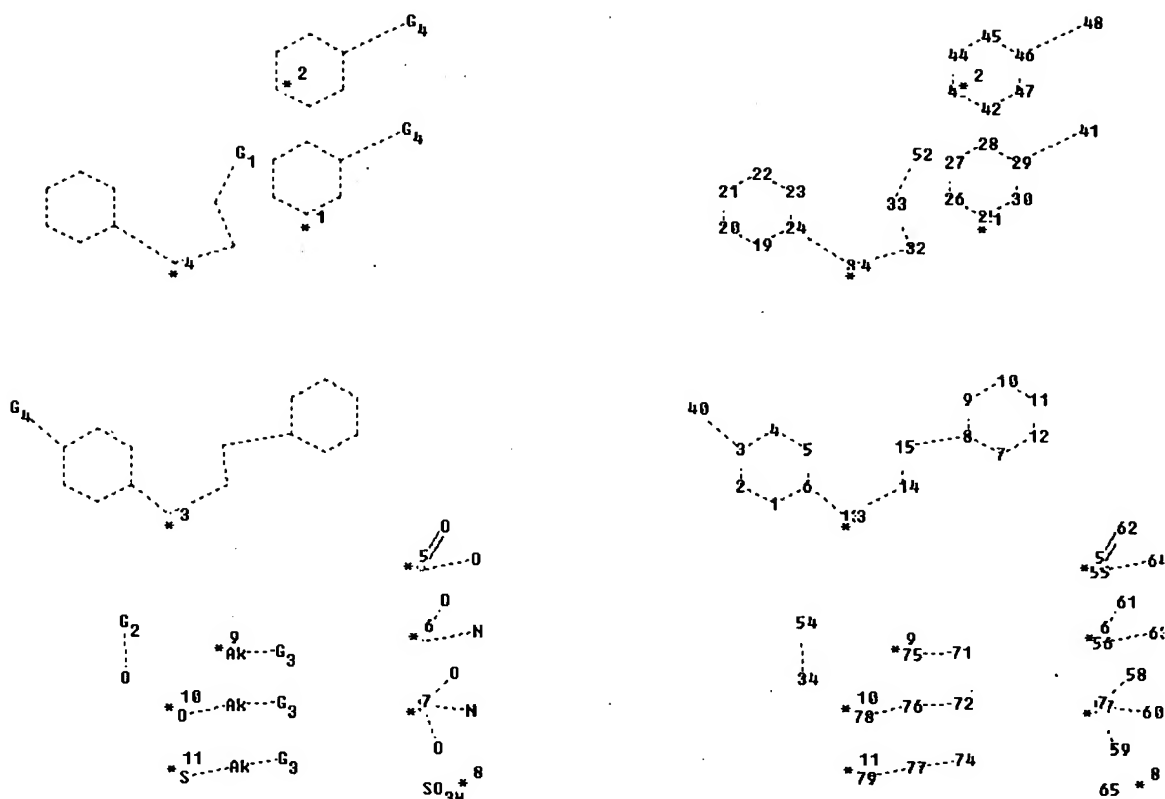
Connectivity :

1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC
ring/chain
4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
7:3 X maximum
RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X
maximum RC ring/chain
11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC
ring/chain 14:3
X maximum RC ring/chain 15:3 X maximum RC ring/chain 19:3 X maximum RC ring/chain
20:3 X maximum
RC ring/chain 21:3 X maximum RC ring/chain 22:3 X maximum RC ring/chain 23:3 X
maximum RC ring/chain
24:3 E exact RC ring/chain 25:3 X maximum RC ring/chain 26:3 X maximum RC
ring/chain 27:3
X maximum RC ring/chain 28:3 X maximum RC ring/chain 29:3 X maximum RC ring/chain
30:3 X maximum
RC ring/chain 31:3 E exact RC ring/chain 32:3 X maximum RC ring/chain 33:3 X
maximum RC ring/chain
34:1 E exact RC ring/chain 42:3 X maximum RC ring/chain 43:3 X maximum RC
ring/chain 44:3
X maximum RC ring/chain 45:3 X maximum RC ring/chain 47:3 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS
34:CLASS 40:CLASS
41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 52:CLASS
54:CLASS

L5 2322 SEA FILE=REGISTRY SSS FUL L3 AND L1
L6 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation:
Uploading L6.str



chain nodes :

13 14 15 31 32 33 34 40 41 48 52 54 55 56 57 58 59 61 62 64 65
71 72 74 75 76 77 78 79

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 19 20 21 22 23 24 25 26 27 28 29
30 42 43 44 45 46 47

ring/chain nodes :

60 63

chain bonds :

3-40 6-13 8-15 13-14 14-15 24-31 29-41 31-32 32-33 33-52 34-54 46-48
55-62 55-64 56-61 56-63 57-58 57-59 57-60 71-75 72-76 74-77 76-78 77-79

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24 20-21
21-22 22-23 23-24 25-26 25-30 26-27 27-28 28-29 29-30 42-43 42-47 43-44
44-45 45-46
46-47

exact/norm bonds :

1-2 1-6 2-3 3-4 3-40 4-5 5-6 6-13 7-8 7-12 8-9 8-15 9-10 10-11 11-12
13-14 14-15 19-20 19-24 20-21 21-22 22-23 23-24 24-31 25-26 25-30 26-27
27-28 28-29
29-30 29-41 31-32 32-33 33-52 34-54 42-43 42-47 43-44 44-45 45-46 46-47
46-48 55-62
55-64 56-61 56-63 57-58 57-59 57-60 71-75 72-76 74-77 76-78 77-79

G1: [*1], [*2]

G2:[*3],[*4]

G3:[*5],[*6],[*7],[*8]

G4:[*9],[*10],[*11]

Connectivity :

1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC ring/chain
 4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
 7:3 X maximum RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X maximum RC ring/chain
 11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC ring/chain 14:3 X maximum RC ring/chain
 15:3 X maximum RC ring/chain 19:3 X maximum RC ring/chain 20:3 X maximum RC ring/chain
 21:3 X maximum RC ring/chain 22:3 X maximum RC ring/chain 23:3 X maximum RC ring/chain
 24:3 E exact RC ring/chain 25:3 X maximum RC ring/chain 26:3 X maximum RC ring/chain 27:3 X maximum RC ring/chain
 28:3 X maximum RC ring/chain 29:3 X maximum RC ring/chain 30:3 X maximum RC ring/chain
 31:3 E exact RC ring/chain 32:3 X maximum RC ring/chain 33:3 X maximum RC ring/chain
 34:1 E exact RC ring/chain 42:3 X maximum RC ring/chain 43:3 X maximum RC ring/chain 44:3 X maximum RC ring/chain
 45:3 X maximum RC ring/chain 47:3 X maximum RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom
 23:Atom 24:Atom
 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS
 34:CLASS 40:CLASS
 41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 52:CLASS
 54:CLASS
 55:CLASS 56:CLASS 57:CLASS 58:CLASS 59:CLASS 60:CLASS 61:CLASS 62:CLASS
 63:CLASS 64:CLASS
 65:CLASS 71:CLASS 72:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS 78:CLASS
 79:CLASS

L8 68 SEA FILE=REGISTRY SUB=L5 SSS FUL L6
 L9 12 SEA FILE=ZCAPLUS ABB=ON PLU=ON L8

=> s L9 not L25
 L26 9 L9 NOT L25

=> file beilstein

FILE 'BEILSTEIN' ENTERED AT 13:15:02 ON 01 OCT 2007
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FILE LAST UPDATED ON September 26, 2007

FILE COVERS 1771 TO 2007.

*** FILE CONTAINS 10.119,480 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

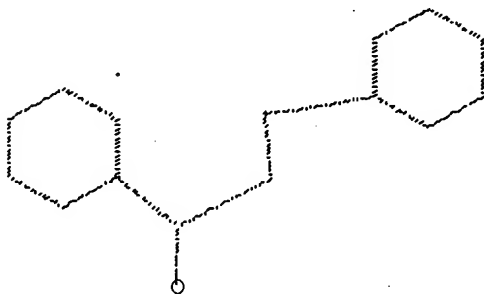
>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

 * PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
 * SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
 * ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
 * ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
 * FOR PRICE INFORMATION SEE HELP COST *

NEW

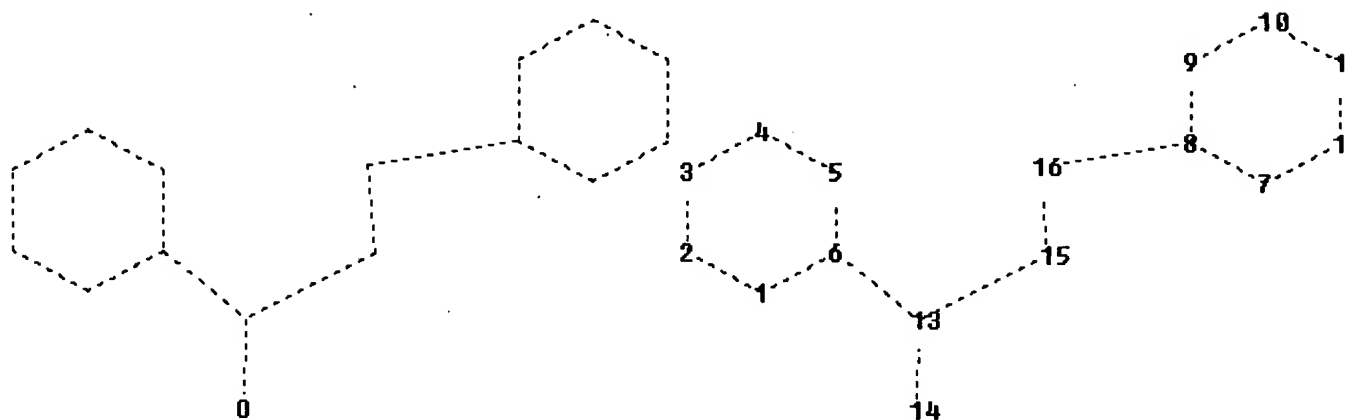
* **PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.**
 * **NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.**

=> d stat que L13
 L1 STR



Structure attributes must be viewed using STN Express query preparation:
 Uploading L1.str

10/520079



chain nodes :

13 14 15 16

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

6-13 8-16 13-14 13-15 15-16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 6-13 7-8 7-12 8-9 8-16 9-10 10-11 11-12 13-14
13-15 15-16

Connectivity :

1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC
ring/chain

4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
7:3 X maximum

RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X
maximum RC ring/chain

11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC
ring/chain 14:1

E exact RC ring/chain 15:3 X maximum RC ring/chain 16:3 X maximum RC ring/chain
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

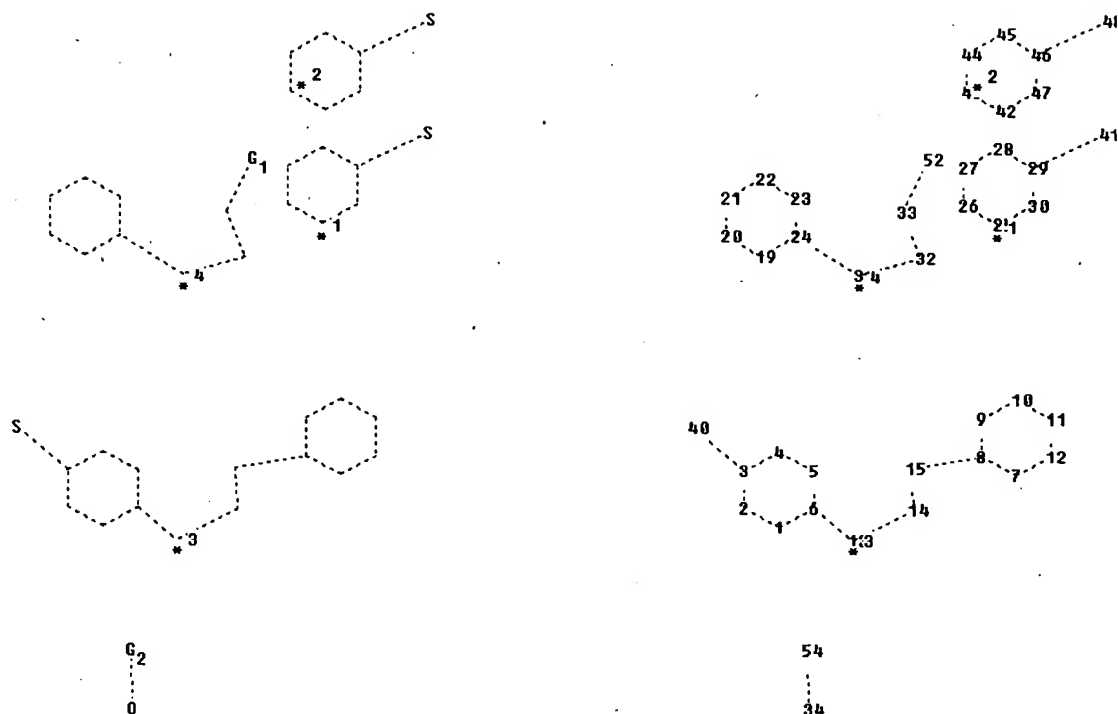
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS

L3

STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:
Uploading L3.str



chain nodes :

13 14 15 31 32 33 34 40 41 48 52 54

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 19 20 21 22 23 24 25 26 27 28 29
30 42 43 44 45 46 47

chain bonds :

3-40 6-13 8-15 13-14 14-15 24-31 29-41 31-32 32-33 33-52 34-54 46-48

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24 20-21
21-22 22-23 23-24 25-26 25-30 26-27 27-28 28-29 29-30 42-43 42-47 43-44
44-45 45-46
46-47

exact/norm bonds :

1-2 1-6 2-3 3-4 3-40 4-5 5-6 6-13 7-8 7-12 8-9 8-15 9-10 10-11 11-12
13-14 14-15 19-20 19-24 20-21 21-22 22-23 23-24 24-31 25-26 25-30 26-27
27-28 28-29
29-30 29-41 31-32 32-33 33-52 34-54 42-43 42-47 43-44 44-45 45-46 46-47
46-48

G1:[*1],[*2]

G2:[*3],[*4]

Connectivity :

1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC

ring/chain

4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain 7:3 X maximum

RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X maximum RC ring/chain

11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC ring/chain 14:3

X maximum RC ring/chain 15:3 X maximum RC ring/chain 19:3 X maximum RC ring/chain 20:3 X maximum

RC ring/chain 21:3 X maximum RC ring/chain 22:3 X maximum RC ring/chain 23:3 X maximum RC ring/chain

24:3 E exact RC ring/chain 25:3 X maximum RC ring/chain 26:3 X maximum RC ring/chain 27:3

X maximum RC ring/chain 28:3 X maximum RC ring/chain 29:3 X maximum RC ring/chain 30:3 X maximum

RC ring/chain 31:3 E exact RC ring/chain 32:3 X maximum RC ring/chain 33:3 X maximum RC ring/chain

34:1 E exact RC ring/chain 42:3 X maximum RC ring/chain 43:3 X maximum RC ring/chain 44:3

X maximum RC ring/chain 45:3 X maximum RC ring/chain 47:3 X maximum RC ring/chain Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom

25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS

34:CLASS 40:CLASS

41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 52:CLASS

54:CLASS

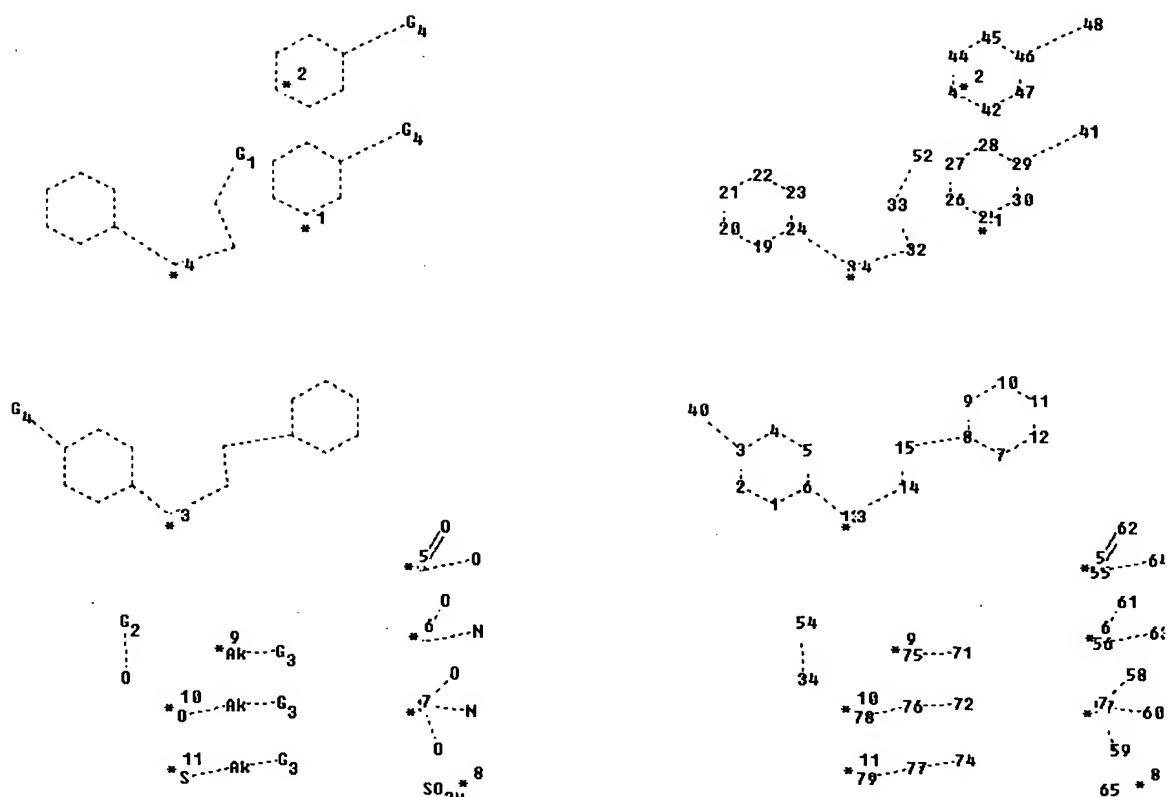
L6

STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation:

Uploading L6.str



chain nodes :

13 14 15 31 32 33 34 40 41 48 52 54 55 56 57 58 59 61 62 64 65
71 72 74 75 76 77 78 79

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 19 20 21 22 23 24 25 26 27 28 29
30 42 43 44 45 46 47

ring/chain nodes :

60 63

chain bonds :

3-40 6-13 8-15 13-14 14-15 24-31 29-41 31-32 32-33 33-52 34-54 46-48
55-62 55-64 56-61 56-63 57-58 57-59 57-60 71-75 72-76 74-77 76-78 77-79

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24 20-21

21-22 22-23 23-24 25-26 25-30 26-27 27-28 28-29 29-30 42-43 42-47 43-44
44-45 45-46

46-47

exact/norm bonds :

1-2 1-6 2-3 3-4 3-40 4-5 5-6 6-13 7-8 7-12 8-9 8-15 9-10 10-11 11-12
13-14 14-15 19-20 19-24 20-21 21-22 22-23 23-24 24-31 25-26 25-30 26-27

27-28 28-29

29-30 29-41 31-32 32-33 33-52 34-54 42-43 42-47 43-44 44-45 45-46 46-47

46-48 55-62

55-64 56-61 56-63 57-58 57-59 57-60 71-75 72-76 74-77 76-78 77-79

G1: [*1], [*2]

10/520079

G2:[*3],[*4]

G3:[*5],[*6],[*7],[*8]

G4:[*9],[*10],[*11]

Connectivity :

1:3 X maximum RC ring/chain 2:3 X maximum RC ring/chain 3:3 X maximum RC
ring/chain
4:3 X maximum RC ring/chain 5:3 X maximum RC ring/chain 6:3 E exact RC ring/chain
7:3 X maximum
RC ring/chain 8:3 E exact RC ring/chain 9:3 X maximum RC ring/chain 10:3 X
maximum RC ring/chain
11:3 X maximum RC ring/chain 12:3 X maximum RC ring/chain 13:3 E exact RC
ring/chain 14:3
X maximum RC ring/chain 15:3 X maximum RC ring/chain 19:3 X maximum RC ring/chain
20:3 X maximum
RC ring/chain 21:3 X maximum RC ring/chain 22:3 X maximum RC ring/chain 23:3 X
maximum RC ring/chain
24:3 E exact RC ring/chain 25:3 X maximum RC ring/chain 26:3 X maximum RC
ring/chain 27:3
X maximum RC ring/chain 28:3 X maximum RC ring/chain 29:3 X maximum RC ring/chain
30:3 X maximum
RC ring/chain 31:3 E exact RC ring/chain 32:3 X maximum RC ring/chain 33:3 X
maximum RC ring/chain
34:1 E exact RC ring/chain 42:3 X maximum RC ring/chain 43:3 X maximum RC
ring/chain 44:3
X maximum RC ring/chain 45:3 X maximum RC ring/chain 47:3 X maximum RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
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23:Atom 24:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS
34:CLASS 40:CLASS
41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 52:CLASS
54:CLASS
55:CLASS 56:CLASS 57:CLASS 58:CLASS 59:CLASS 60:CLASS 61:CLASS 62:CLASS
63:CLASS 64:CLASS
65:CLASS 71:CLASS 72:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS 78:CLASS
79:CLASS

L11 383 SEA FILE=BEILSTEIN SSS FUL L1 AND L3
L13 5 SEA FILE=BEILSTEIN SUB=L11 SSS FUL L6

100.0% PROCESSED 383 ITERATIONS 5 ANSWERS
SEARCH TIME: 00.00.01

=> dup rem L26 L13

DUPLICATE IS NOT AVAILABLE IN 'BEILSTEIN'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
FILE 'ZCAPLUS' ENTERED AT 13:15:17 ON 01 OCT 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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